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MODELING AND UNCERTAINTY QUANTIFICATION OF PARTICULATE COMPOSITE MATERIALS

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Nomenclature:

J	Compliance
A	Linear parameter in creep model
n	Exponential parameter in creep model
t	Time
Z	Z-statistic from uniform normal distribution
μ	Population mean
σ	Population standard deviation
$\overline{X}$	Sample mean
n	Sample size

ABSTRACT

Particulate composites are a growing material class that offers various advantages and disadvantages by blending the strengths and weaknesses of their constituents. Although typically not designed for structural applications, their dynamic responses are still of interest and should be investigated, modeled, and validated over the intended design space. For this study, the creep behavior of a mock explosive 900-30 and a fiber wood composite, ChoiceDek®, was investigated in order to characterize the long-term mechanical response. Based on similar materials, a viscoelastic creep models was identified. A design of experiments was developed, and creep tests were conducted. Finally, validation experiments were performed in order to assess the accuracy and adequacy of the analytical model. After performing this procedure on a limited sample size there is an indication that it is possible to predict creep behavior at 200 hrs of using data collected from 20-hrs experiments. It was also found that the creep behavior of ChoiceDeck® is dissimilar from the 900-30 material, but the mock 900-30 behaves similarly to samples of PBX 9501, a high explosive material the 900-30 is modeled after.

1. INTRODUCTION

Many forms of high explosives (HE) and solid propellants are of the material class known as particulate composites. In both cases, crystals with desired energetic properties are held together by a binder, which provides improved structural properties. The properties of the crystals that allow the material to release large quantities of energy have been well analyzed and documented. However, little effort has been dedicated to studying the mechanical properties of the particulate composites, as they were not intended for structural settings. There are several applications such as rockets where the composite material, to some extent, becomes part of the structural makeup of the system housing it. Forces are inevitably transferred onto the material, making the understanding of how this material behaves critical when designing the system. Additionally, it is common for such systems to lay in storage for long periods of time (perhaps even decades) before being used. This makes the creep characteristics a fundamental part of assessing the readiness and reliability of the system throughout its lifespan. Solid fuel may cope well with internal stresses when the rocket is first built, but may not deliver the same performance after it has changed because of creep. Additionally, the deformation that accompanies creep can change the center of mass and moments of inertia of the rocket, which can affect flight dynamics. Thus, there is a need to be able to model and predict the creep behavior of these particulate composites for long time periods. This study is the beginning of an effort to determine and validate creep models for these types of particulate composites.

Because of the dangerous nature of HE and the subsequent high cost of testing such a material, non-energetic particulate composites were considered first. Two non-energetic particulate composites were considered for this study, the mock explosive, 900-30, and the wood composite, ChoiceDek®. Besides the lower cost of testing associated with the non-energetic particulate composites, it is useful to know how well these materials represent actual HE for other testing applications. Thus, the goal of this study was two fold. The first goal was to develop rigorous testing and analysis for determining and validating creep models for particulate composites. The second goal was to determine how well the non-energetic composites approximate the mechanical behavior of HE. The experimental setup and the design of experiments are presented first followed by a discussion of the results and analysis techniques.

2. EXPERIMENTAL PROCEDURE

The creep experiments for this study were conducted on a bench-top creep frame, Figure 1. The creep frame consisted of two aluminum plates that held and compressed a sample. The load was provided by the mechanical advantage of a cantilever through a ball bearing to the top aluminum plate. The bottom aluminum plate was connected to a load cell that recorded the load in the system, and the load cell was threaded to an additional aluminum block that rested on a base plate through a ball bearing. Two extensometers were used to measure the relative displacement of the top and bottom plates, and the strain in the sample was calculated from the average displacement measurement from the two extensometers. The averaging of the two extensometers removed the effect of nonparallel displacement of the plates.

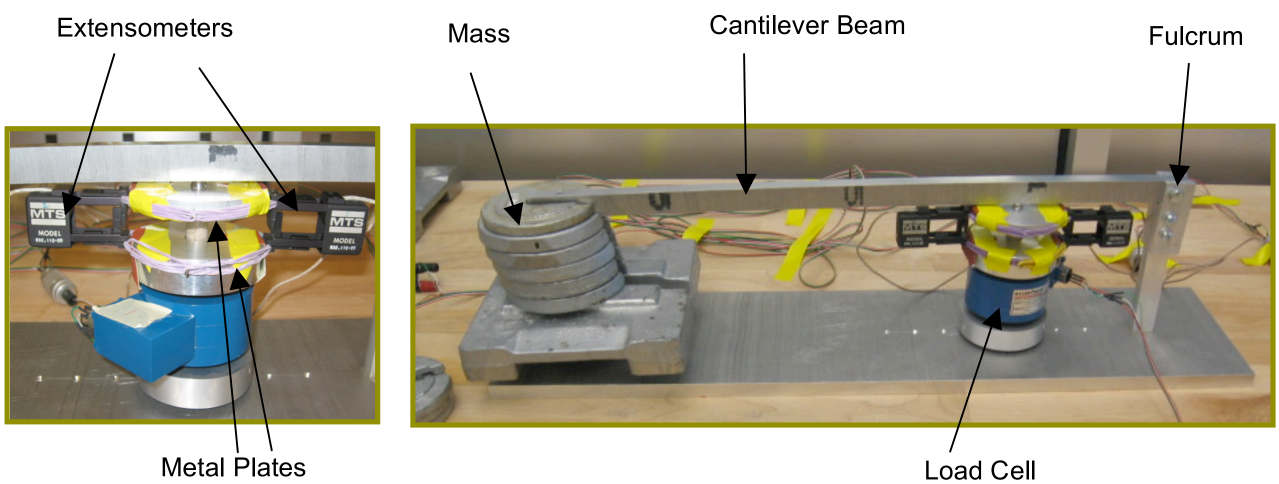

Figure 1 –Experimental Setup

The extensometer and the load cell voltage outputs were recorded using a National Instrument’s system equipped with LABview software. The system was configured to sample at 60Hz and to compute an average every second. The computed averages were used for the data analysis. Due to noise in the extensometer signal, a low pass filter (30Hz) was included to remove the harmonic effects of ambient noise.

Temperature measurements in the testing room indicated that temperature changes were insignificant throughout all of the experiments, at approximately ±0.25°F maximum.

For each test a new sample was used. The sample was placed in the creep frame, the data acquisition system was started, and then the load was applied.

2.1 Design of Experiments

The creep behavior of polymers is influenced by time, temperature, and in some cases the applied load (i.e. stress). However, without a sufficiently large environmental chamber, only the applied load and the duration of the test were varied for these experiments. A full-factorial Design of Experiments (DoE) was created using the software JMP™. The DoE considered three different timescales, 2 hours, 20 hours, and 200 hours, and two stress levels, 1.6 MPa and 3.2 MPa. Three tests were performed for each combination of stress and time for a total of 18 tests. The order of the tests was randomized; however, due to time constraints most of the 200 hr tests were pushed to the end to maximize the number of completed tests.

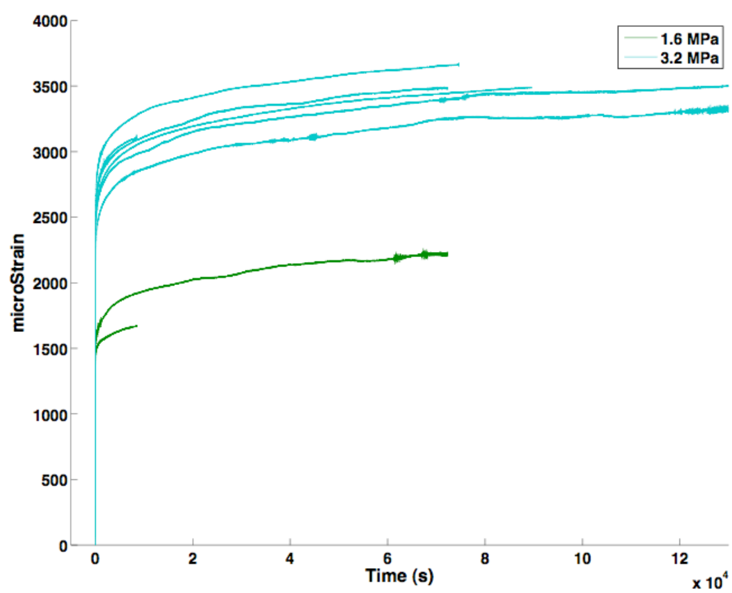

Figure 1 - Strain for ChoiceDek experimental tests.

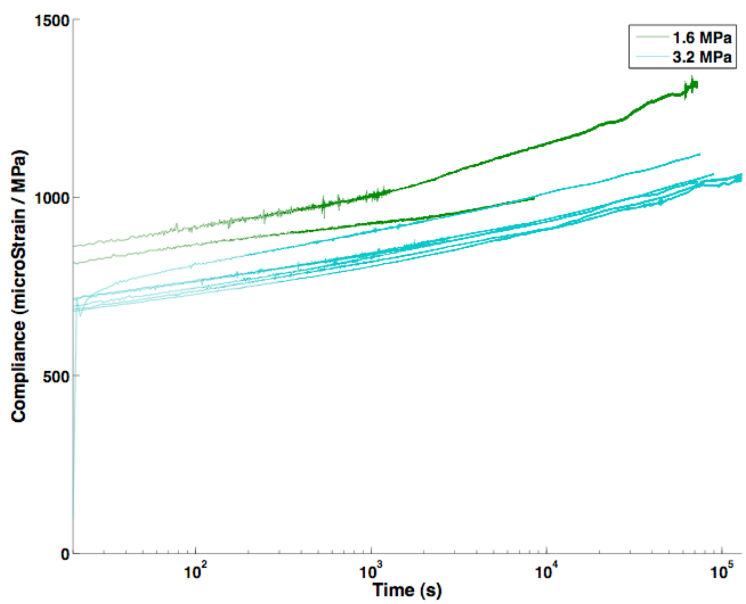

Figure 2 - Compliance for the ChoiceDek experiments.

3. RESULTS AND DISCUSSION

Time constraints on this project ultimately permitted only two 200 hour tests to be conducted on the ChoiceDek®, and only a handful of 20 hour samples of the Mock HE 900-30 were tested. The model development of the ChoiceDek® is presented first, and then the comparison with mock 900-30 and PBX 9501.

3.1 ChoiceDek® Model Development

The wood composite, ChoiceDek®, is composed of 50% wood fibers and 50% polyethylene (high and low density). With such a large fraction of the volume being polyethylene, the creep behavior of the wood composite was expected to be similar to plain polyethylene, which has a nonlinear creep response. [3],[5]

The strain versus time response obtained from the constant stress creep experiments is shown in Figure 2. Two distinct strain responces become apparent for the loading conditions, with stresses of 1.6MPa and 3.2MPa on the samples. Unfortunately, of the 12 tests conducted for the two stress levels and the lower two time lengths, only six tests were without anomalies. For several of the tests at least one of extensometers slipped and for others there were other abnormal jumps in the data. A plot of the compliance, Figure 3, indicates the samples that experienced a higher load had a lower compliance. However, the small number of tests and spread in the data due to the heterogeneous nature of the sample do not allow any conclusions to be made.

For simplicity, the creep compliance data was fit to a simple power law:

$$J = At^{n} \tag{1}$$

Figure 3 shows an example of the ability of the power law to fit the ChoiceDek® creep data, red line. However, there is a nontrivial difference between the various compliance curves. To accurately represent this amount of spread for future analyses, this uncertainty must be quantified and considered in the model validation.

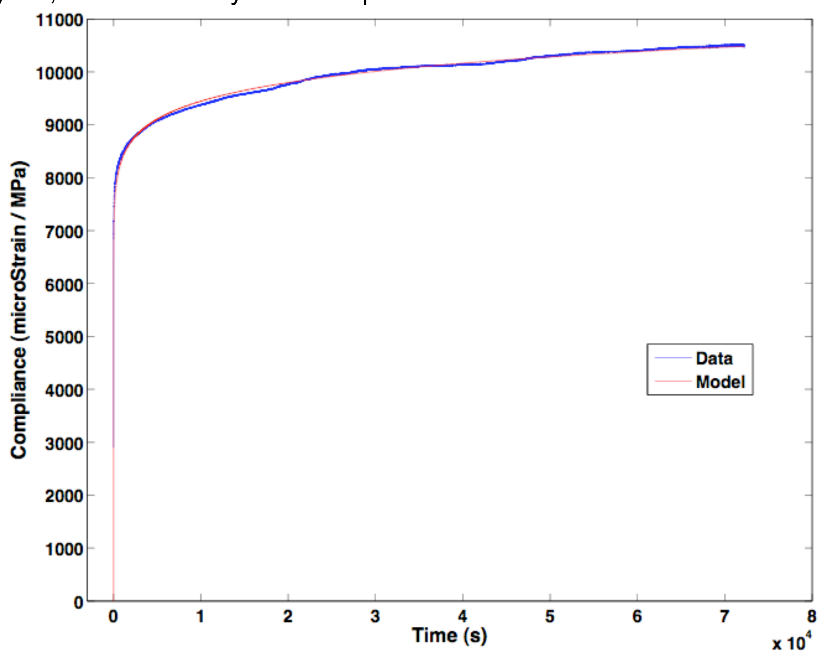

Figure 3 - Power law model compared to experimental data.

3.2 Uncertainty Quantification

In this study, uncertainty inherent in the creep process was quantified using a probabilistic approach that defined distributions on the creep behavior as time progresses. This method allows a model to be developed for use in predicting long-term creep behavior with associated uncertainty. As an initial validation, the model along with the probabilistic information was used to extrapolate compliance at longer time scales, which was compared to the results of a long-term creep test.

In order to construct uncertainty distributions, the compliance sample mean and standard deviation statistics for the experimental ChoiceDek® creep data were calculated at several points in time. For ease of statistical analysis, it was assumed that the experimental results were normally distributed, allowing the mean and standard deviation to define normal probability density functions (PDF) at the sampled points in time. Even with a small number of samples (*n=6*), normal probability plots and the Shapiro-Wilks test supported the normal assumption.

The power law model was then fit to samples drawn from the compliance PDFs, allowing the compliance uncertainty to be modeled through time. The first step in this process was to sample each time slice PDF using a Latin hypercube sampling method with 100 bins. The samples from each bin throughout time were then fit to obtain 100 compliance models of the form of Equation (1). These compliance curves could then be used to predict the range of compliance the material may exhibit for time lengths much greater than the 20 hours the test data covered.

3.3 ChoiceDek® Model Validation

In order to perform a validation of the compliance model, the compliance and associated uncertainty was predicted at 200 hours, a factor of ten longer than any previous test. Experimental creep tests were then performed on the ChoiceDek® for 200 hours at both 1.6 and 3.2 MPa stress levels. A qualitative comparison between the test and model has been shown in Figure 4. This figure shows that the compliance test data falls within the calculated uncertainty of the model at 200 hours.

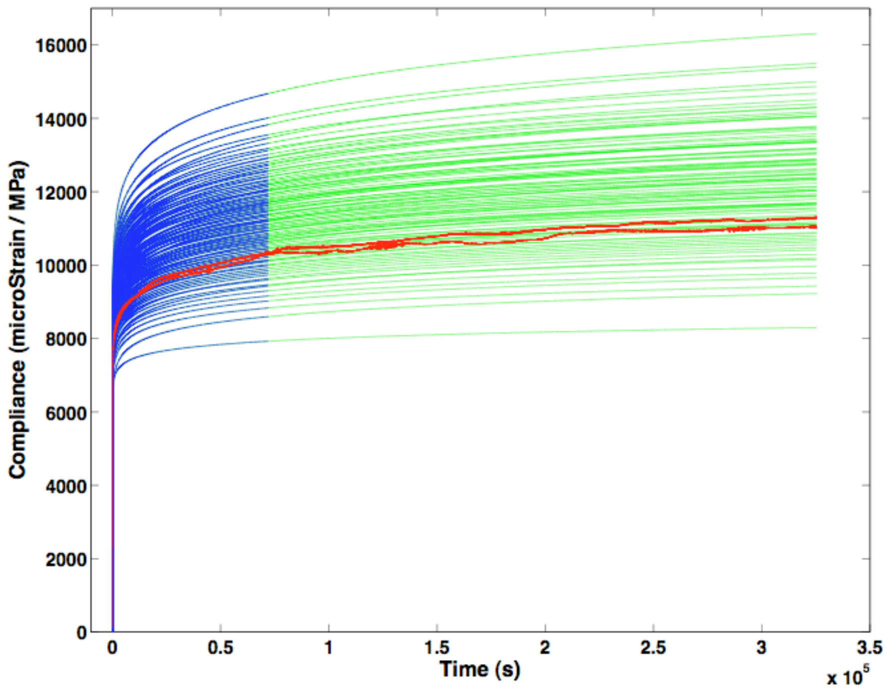

Figure 4 - Compliance model prediction (green) compared to 200-hour validation tests (red) for the ChoiceDek material based on 20-hour test realizations (blue).

A quantitative metric of validation was also implemented to support the qualitative comparison. In this validation, a simple hypothesis test on the mean is used. Assuming the 100 compliance curves form a population, the null hypothesis (H_O) asks if the experimental data are drawn from the model population. If H_O is rejected, then the model can be rejected as an accurate representation of the long-term creep behavior. If H_O is accepted, then there is no evidence that the experimental data differs from the model, and then model is therefore valid.

To perform the hypothesis test, the Z Statistic is first computed for a single point in time, 200 hours in this instance:

$$Z_0 = \frac{\overline{X} - \mu_0}{\frac{\sigma}{\sqrt{n}}} \tag{2}$$

Where, Z_o is the Test Statistic, $\overline{X}$ is the experimental mean, μ_o is the model mean, σ is the standard deviation of the model, and *n* is the number of experimental samples. Z_0 for the 200 hr samples was calculated to be -1.1132. Using the standard normal cumulative distribution function a two tailed test is performed with 95% confidence (α=0.05), the required Z score to reject H_O would be Z<-1.96, therefore the model is not rejected and is considered valid.

3.4 Mock HE 900-30 Comparison

Three 20 hour experiments at 1.6 MPa were performed on the Mock HE 900-30. To compare the 900-30 results to the ChoiceDek®, another hypothesis test was performed. Here the H_O is the ChoiceDek® model is an accurate representation of the 900-30 compliance. The three samples were compared with the model at t=20 hours and Z_o was calculated to be 14.9378, where a Z_o>1.96 would reject the model. Therefore, the ChoiceDek® model is not an accurate representation of the 900-30 compliance behavior. A plot of this test can be seen in Figure 5.

Next, the 900-30 Mock HE was qualitatively compared with PBX 9501 HE data previously collected at LANL. Figure 6 shows that the PBX 9501 compliance for 1.5 MPa tests is similar to the behavior of the 900-30 at 1.6 MPa. These results are encouraging, and provide evidence that the 900-30 is indeed a decent creep mock for the energetic 9501.

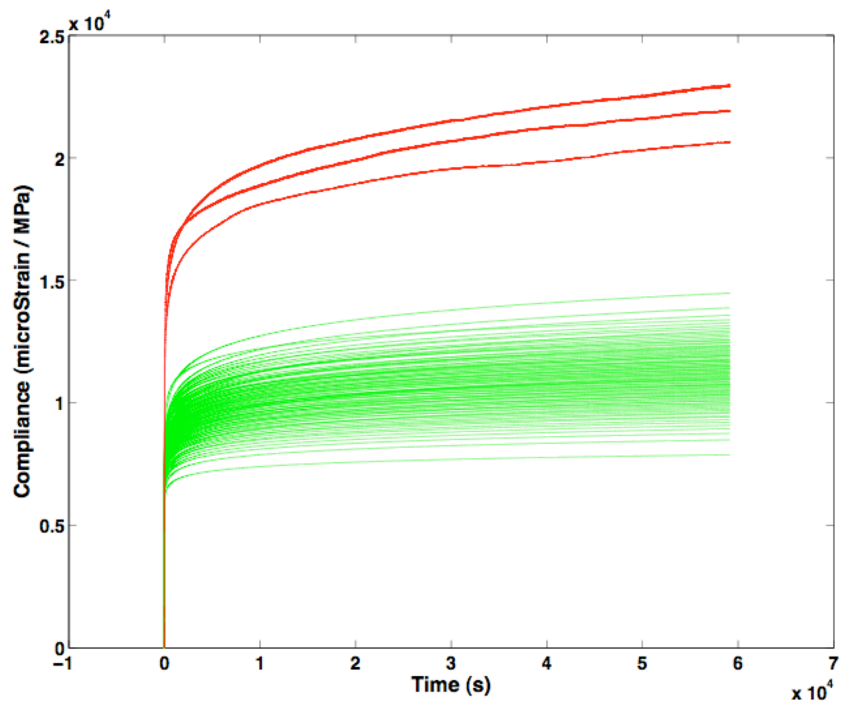

Figure 5 - 900-30 compliance (red) results compared to predicted values (green) from model.

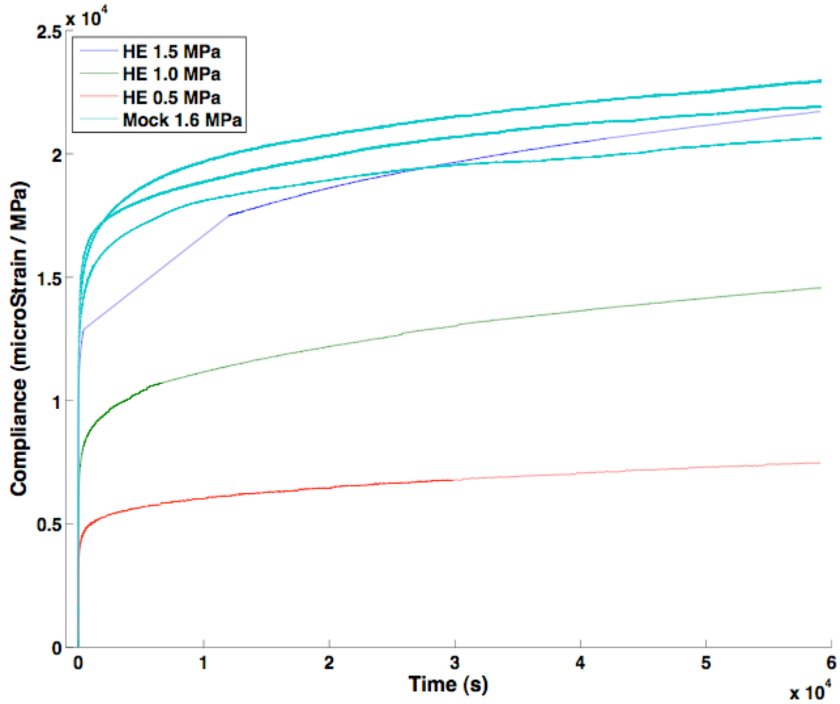

Figure 6 - Qualitative comparison between compliance of 900-30 Mock HE and PBX 9501 HE.

4.1 CONCLUSIONS

The purpose of this project was to answer three questions. First, can creep compliance be predicted over the long term such as 200 hours using experimental data taken over only a short term such as 20 hours? Next, can ChoiceDek® be used as an inexpensive surrogate material for a material such as Mock 900-30? Finally, if ChoiceDek® is not a good surrogate will Mock 900-30 perform adequately as a non-energetic substitute for PBX-9501 in mechanical simulations. A rigorous model validation approach was applied to investigate these three questions though the quantity of the data limits the usefulness of the results.

Using the ChoiceDek® surrogate material, it was shown that creep models derived from 20 hour experiments can be used to predict creep compliance as far out as 200 hours. This suggests that it is reasonable to extrapolate creep behavior as much as an order of magnitude in time.

It was shown that ChoiceDek® is not a good surrogate for Mock 900-30. Qualitatively there is a large disparity between the compliance of ChoiceDek® and Mock 900-30. The Mock 900-30 is approximately twice as compliant as the ChoiceDek®. Quantitatively, the hypothesis test resulted in a test statistic of 14.9 which is much greater than the rejection threshold of 1.96. Therefore, ChoiceDek® cannot be usedas an inexpensive surrogate for mock 900-30.

Finally, qualitative evidence suggests that Mock 900-30 is a good structural surrogate for PBX-9501 when creep behavior is of interest. A rigorous hypothesis testing was not performed in answering this question because the quantity of data was too limited. However, the 1.6 MPa creep compliance for Mock 900-30 does qualitatively appear to closely match 1.5 MPa creep compliance for PBX-9501. With further experimentation and a rigorous model validation it is likely the Mock 900-30 can be used as a safer alternative to PBX-9501 in structural experiments.

5.1 Future Work

This research demonstrates a method of parameterizing creep behavior of materials, quantifying the uncertainty in the parameters, and validating the material model over a particular domain of interest. This method development and demonstration is the major contribution of the work. The weakness of this research is the quantity of data. The largest sample set, which was the ChoiceDek® material, only included 6 experiments. There were 3 experiments performed with the Mock 900-30, and 1 data set was provided for the PBX-9501 at a comparable stress level. The results and usefulness of this work will be greatly expanded by performing additional experiments. It will likely be unfruitful to perform additional ChoiceDek® creep experiments; however, there will be great benefit from performing more creep experiments with Mock 900-30 and obtaining more data for PBX-9501. In addition to improving the hypothesis testing, stress dependence can be further investigated using several more stress levels.

6.1 Acknowledgements
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REFERENCES

[1] Callister, W., “Composites,” in *Materials Science and Engineering an Introduction*, Fourth Edition. New York: John Wiley & Sons, Inc., 1997. pp. 510-517

[2] Guide for Verification and Validation in Computational Solid Mechanics, *American Society of Mechanical Engineers*, March 29, 2006

[3] Lai, J and Bakker, A. (1995). “Analysis of the Non-Linear Creep of High-Density Polyethylene,” Polymer 36, p93-99.

[4] Pack, R., “Chemical Kinetics of the Aging of Estane 5703 in PBX 9501. I. First Preliminary Predictions,” Theoretical Division T-12, Los Alamos National Laboratory

[5] Rand, J.L., Henderson, J.K. and Grant, D.B. (1996). “Nonlinear Behavior of Linear Low-Density Polyethylene,” Poly. Eng. Sci. 36, p1058-1064.